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Uniform asymptotic approximations for incomplete Riemann Zeta functions

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Dedicated to Roderick Wong on the occasion of his 60th birthday

Abstract

An incomplete Riemann Zeta function $Z_1(\alpha, x)$ is examined, along with a complementary incomplete Riemann Zeta function $Z_2(\alpha, x)$. These functions are defined by $Z_1(\alpha, x) = \{(1 - 2^{1-\alpha})\Gamma(\alpha)\}^{-1} \int_0^x t^{\alpha-1}(e^t + 1)^{-1}\, dt$ and $Z_2(\alpha, x) = \zeta(\alpha) - Z_1(\alpha, x)$, where $\zeta(\alpha)$ is the classical Riemann Zeta function. $Z_1(\alpha, x)$ has the property that $\lim_{x\to\infty} Z_1(\alpha, x) = \zeta(\alpha)$ for $\operatorname{Re} \alpha > 0$ and $\alpha \neq 1$. The asymptotic behaviour of $Z_1(\alpha, x)$ and $Z_2(\alpha, x)$ is studied for the case $\operatorname{Re} \alpha = \sigma > 0$ fixed and $\operatorname{Im} \alpha = \tau \to \infty$, and using Liouville–Green (WKBJ) analysis, asymptotic approximations are obtained, complete with explicit error bounds, which are uniformly valid for $0 \leqslant x < \infty$.

MSC: Primary 33E20; Secondary 11M06, 34E20

1. Introduction

It is well known that the Riemann Zeta function has the integral representation

$$\zeta(\alpha) = \frac{1}{(1 - 2^{1-\alpha})\Gamma(\alpha)} \int_0^\infty \frac{t^{\alpha-1}}{e^t + 1}\, dt, \tag{1.1}$$

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which converges and defines $\zeta(\alpha)$ for all $\operatorname{Re}\alpha > 0$ (except at the pole $\alpha = 1$). With this definition in mind, we introduce an incomplete Riemann Zeta function

$$Z_1(\alpha, x) = \frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)} \int_0^x \frac{t^{\alpha-1}}{e^t+1}\,dt \quad (\operatorname{Re}\alpha > 0,\ \alpha \neq 1), \tag{1.2}$$

along with a complementary incomplete Riemann Zeta function

$$Z_2(\alpha, x) = \frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)} \int_x^\infty \frac{t^{\alpha-1}}{e^t+1}\,dt \quad (\alpha \neq 1). \tag{1.3}$$

In the integrands of (1.2) and (1.3) the principal branch of t^α is taken. Here and throughout we assume that x is real with $0 \leqslant x < \infty$, and from now on that α is not equal to 1, and satisfies

$$\alpha = \sigma + i\tau, \quad \sigma > 0, \quad 0 \leqslant \tau < \infty. \tag{1.4}$$

From (1.1)–(1.3) it is evident that for $0 \leqslant x < \infty$

$$\zeta(\alpha) = Z_1(\alpha, x) + Z_2(\alpha, x). \tag{1.5}$$

Therefore $Z_1(\alpha, x)$ and $Z_2(\alpha, x)$ are linearly independent (as functions of x) if and only if $\zeta(\alpha) \neq 0$. The definitions (1.2) and (1.3) are analogous to those of the incomplete and complementary incomplete Gamma functions

$$\gamma(\alpha, x) = \int_0^x t^{\alpha-1} e^{-t}\,dt \quad (\operatorname{Re}(\alpha) > 0), \tag{1.6}$$

$$\Gamma(\alpha, x) = \int_x^\infty t^{\alpha-1} e^{-t}\,dt, \tag{1.7}$$

which of course satisfy $\Gamma(\alpha) = \gamma(\alpha, x) + \Gamma(\alpha, x)$.

Kölbig [6,7] undertook a numerical study of the trajectory of the zeros of the incomplete Riemann Zeta function (1.2) in the complex α plane, with x regarded as a real parameter. However, he remarked that the expansions he employed suffered from numerical instabilities as τ increased. For instance, in a footnote in [7] Kölbig mentions that it would be interesting to study the zero trajectories near a zero-free Gram interval, the first of these being near $\tau = 282$, but alluded that he was unable to do so as this range was "far beyond the range of the present calculations."

The purpose of this paper is to study the asymptotics of $Z_1(\alpha, x)$ and $Z_2(\alpha, x)$; we shall obtain leading term approximations as $\tau \to \infty$, complete with explicit error bounds. In a subsequent paper we will investigate the case where the argument x is complex, as well as extensions to asymptotic expansions. Our approach here will be via a differential equation: specifically, a straightforward differentiation shows that $y = Z_1(\alpha, x)$ and $y = Z_2(\alpha, x)$ (along with a trivial solution $y = 1$) satisfy the second order linear differential equation

$$\frac{d^2y}{dx^2} = \left\{ \frac{\alpha - 1 - x}{x} + \frac{1}{e^x + 1} \right\} \frac{dy}{dx}. \tag{1.8}$$

Then, removing the first derivative in a standard manner yields

$$\frac{d^2w}{dx^2} = \left[\frac{\alpha^2 - 1}{4x^2} + \frac{(1-\alpha)e^x}{2x(e^x+1)} + \frac{e^x(e^x+2)}{4(e^x+1)^2} \right] w, \tag{1.9}$$

with solutions $w=x^{(1-\alpha)/2}(e^x+1)^{1/2}y$, where $y=Z_1(\alpha,x)$, $y=Z_2(\alpha,x)$, as well as $y=1$. The differential (1.9) will be the main focus of our attention.

We next record the following behaviour of the functions at the endpoints of the x interval:

$$Z_1(\alpha,x)=\frac{x^\alpha}{2\alpha(1-2^{1-\alpha})\Gamma(\alpha)}\{1+O(x)\} \quad (x\to 0), \tag{1.10}$$

$$Z_2(\alpha,x)=\zeta(\alpha)+O(x^\alpha) \quad (x\to 0), \tag{1.11}$$

$$Z_1(\alpha,x)=\zeta(\alpha)+O(x^{\alpha-1}e^{-x}) \quad (x\to \infty), \tag{1.12}$$

$$Z_2(\alpha,x)=\frac{x^{\alpha-1}e^{-x}}{(1-2^{1-\alpha})\Gamma(\alpha)}\{1+O(x^{-1})\} \quad (x\to \infty). \tag{1.13}$$

Thus, provided $\zeta(\alpha)\neq 0$, $Z_1(\alpha,x)$ is recessive and $Z_2(\alpha,x)$ is dominant at $x=0$, with the roles reversed at $x=\infty$. Consider then the following singular eigenvalue problem: for what values of α (with $\mathrm{Re}\,\alpha>0$) does there exist a solution $w=\phi(\alpha,x)$, say, of (1.9) that is recessive at both $x=0$ and $x=\infty$? From (1.10)–(1.13) it is clear that when $\zeta(\alpha)\neq 0$ no such eigensolution exists. However, when $\zeta(\alpha)=0$ we have from (1.3) that $Z_1(\alpha,x)=-Z_2(\alpha,x)$, and consequently

$$\phi(\alpha,x)=x^{(1-\alpha)/2}(e^x+1)^{1/2}Z_1(\alpha,x)=-x^{(1-\alpha)/2}(e^x+1)^{1/2}Z_2(\alpha,x) \tag{1.14}$$

is the unique (to within a multiplicative constant) eigensolution of (1.9) that is recessive at both $x=0$ and ∞: the corresponding eigenvalues α of this singular boundary value problem are of course the non-trivial zeros of $\zeta(\alpha)$. The Riemann Hypothesis is therefore equivalent to the above singular eigenvalue value problem having eigenvalues α which all lie on the critical line $\mathrm{Re}\,\alpha=\frac{1}{2}$.

The importance of the complete Riemann Zeta function $\zeta(\alpha)$ and its zeros is well documented: amongst the many applications in diverse areas, we mention its role in prime number theory, quantum wave physics, and dynamical chaos; see [3]. Whilst there has been an intensive study on the asymptotics of the Riemann Zeta function (for recent results, see [1,2,10,11]), with the exception of [6] and [7] there appear to be few results in the literature (asymptotic or otherwise) for the incomplete Riemann Zeta functions in the above form. In addition to being regarded as eigensolutions of the singular eigenvalue value problem described above, the incomplete Riemann Zeta functions are closely related to several important special functions of mathematical physics and chemistry, specifically Debye [8], Bose-Einstein and Fermi-Dirac functions [4]. We refer the reader to [7] for further details.

The plan of this paper is as follows. In Section 2 we derive a Dirichlet-type asymptotic expansion for $Z_2(\alpha,x)$. This is achieved by expanding the integral (1.3) as a convergent series involving $\Gamma(\alpha,x)$, which in turn is approximated by an established uniform asymptotic approximation. The resulting expansion for $Z_2(\alpha,x)$ is valid for unbounded x, but is not valid for small x due to the lack of uniformity of the re-expansions in terms of the incomplete Gamma function. In Section 3 we construct Liouville–Green (WKBJ) asymptotic solutions to (1.9), complete with explicit error bounds. In Section 4 we match these Liouville–Green solutions with the exact solutions $Z_1(\alpha,x)$ and $Z_2(\alpha,x)$, and by means of a differentiation convert these into a particularly simple form. The resulting approximation for $Z_1(\alpha,x)$ is uniformly valid for $0\leqslant x\leqslant \Omega(\sigma)$ and the approximation for $Z_2(\alpha,x)$ is uniformly valid for $\Omega(\sigma)\leqslant x<\infty$, where $0<\Omega(\sigma)<\infty$ is defined in terms of the Lambert W function. The connection formula (1.5) extends the approximations to all non-negative x. Finally, in Section 5 we give some numerical calculations for the relative errors of our new uniform approximations, and we also demonstrate how the stated intervals of validity can be extended for both $Z_1(\alpha, x)$ and $Z_2(\alpha, x)$.

2. Dirichlet-type expansions

For $x \geqslant \delta > 0$ we can expand the denominator of the integrand of (1.2) as the following geometric series

$$Z_1(\alpha, x) = \frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)} \int_0^x t^{\alpha-1} \sum_{k=1}^{\infty} \mathrm{e}^{-kt}\, \mathrm{d}t, \tag{2.1}$$

and by reversing the integration and summation, and then referring to (1.6), we arrive at the following Dirichlet-type series

$$Z_1(\alpha, x) = \frac{1}{(1-2^{1-\alpha})} \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\gamma(\alpha, kx)}{\Gamma(\alpha) k^{\alpha}} \quad (x \geqslant \delta > 0). \tag{2.2}$$

Likewise, from (1.3) and (1.7),

$$Z_2(\alpha, x) = \frac{1}{(1-2^{1-\alpha})} \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\Gamma(\alpha, kx)}{\Gamma(\alpha) k^{\alpha}} \quad (x \geqslant \delta > 0). \tag{2.3}$$

Consider (2.3). From Temme [12] we have the asymptotic approximation

$$\frac{\Gamma(\alpha, z)}{\Gamma(\alpha)} \sim \frac{1}{2}\mathrm{erfc}(\omega^{1/2}(\alpha, z)) + \frac{\mathrm{e}^{-\omega(\alpha,z)}}{2\sqrt{\pi}} \left\{ \frac{\sqrt{2\alpha}}{z-\alpha} - \frac{1}{\omega^{1/2}(\alpha, z)} \right\} \quad (\alpha \to \infty), \tag{2.4}$$

where

$$\omega(\alpha, z) = z - \alpha - \alpha \ln(z/\alpha). \tag{2.5}$$

The asymptotic expansion (2.4) is valid for $\mathrm{Im}\,\alpha = \tau \to \infty$ uniformly for $0 < z < \infty$. We now set $z = kx$ in (2.4) and then insert into (2.3), which immediately gives

$$Z_2(\alpha, x) \sim \frac{1}{2(1-2^{1-\alpha})} \sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{k^{\alpha}} \left[\mathrm{erfc}(\omega^{1/2}(\alpha, kx)) + \frac{\mathrm{e}^{-\omega(\alpha,kx)}}{\sqrt{\pi}} \left\{ \frac{\sqrt{2\alpha}}{kx-\alpha} - \frac{1}{\omega^{1/2}(\alpha, kx)} \right\} \right], \tag{2.6}$$

as $\tau \to \infty$, uniformly for $0 < \delta \leqslant x < \infty$. We can simplify (2.6) by using the following well-known asymptotic behaviour of the complementary error function

$$\mathrm{erfc}(\omega^{1/2}) \sim \frac{\mathrm{e}^{-\omega}}{\sqrt{\pi\omega}} \left(\omega \to \infty, |\arg(\omega)| \leqslant \frac{3}{2}\pi - \delta_0 < \frac{3}{2}\pi \right). \tag{2.7}$$

With (2.7) in mind, and recalling that $\alpha = \sigma + \mathrm{i}\tau$, we have from (2.5)

$$\omega(\alpha, kx) = kx - \tfrac{1}{2}\pi\tau + \mathrm{i}\tau \ln\{\tau/(ekx)\} + \sigma \ln(\tau/(kx)) + \tfrac{1}{2}\pi\mathrm{i}\sigma + \mathrm{O}(\tau^{-1}) \quad (\tau \to \infty), \tag{2.8}$$

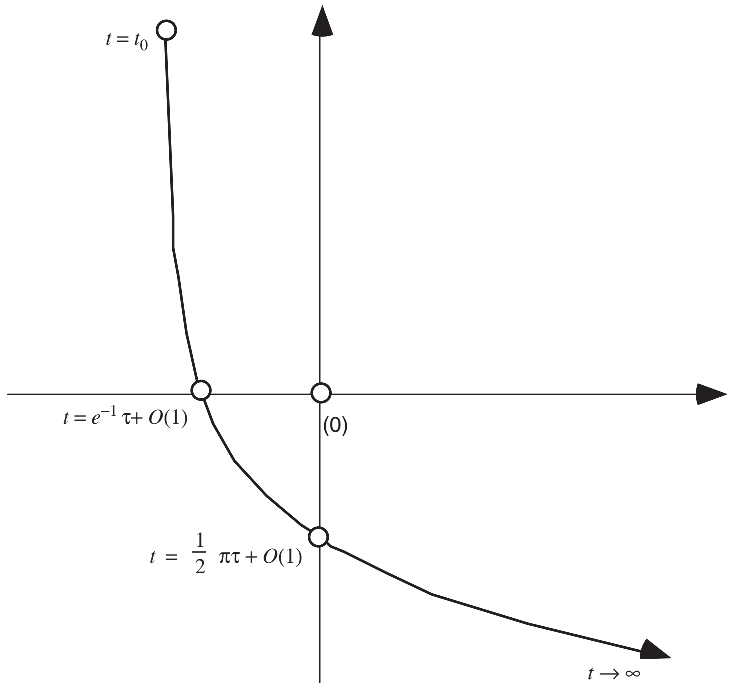

Fig. 1. ω plane.

uniformly for $k \geqslant 1$ and $0 < \delta \leqslant x < \infty$. Using (2.8) it is not difficult to show that $-\frac{3}{2}\pi + \delta_0 \leqslant \arg(\omega) < 0$ ($\delta_0 > 0$), for all $k \geqslant 1$ and x satisfying $0 < \delta \leqslant x < \infty$, provided τ is sufficiently large. Setting $kx = t$ in (2.8), Fig. 1 depicts a typical trajectory of the curve given parametrically by $\omega(\alpha, t)$, for $0 < t_0 \leqslant t < \infty$, where t_0 is arbitrary and $\alpha = \sigma + \mathrm{i}\tau$ is fixed (with τ large). Observe that on this curve ω indeed satisfies $-\frac{3}{2}\pi + \delta_0 \leqslant \arg(\omega) < 0$ (for some fixed $\delta_0 > 0$) (Fig. 1).

Since (2.7) applies for all terms in the series (2.6) we may use it to replace all the erfc terms in the series. Thus, on referring to (2.5), we finally arrive at the simpler form

$$Z_2(\alpha, x) \sim \sqrt{\frac{\alpha}{2\pi}} \frac{1}{(1 - 2^{1-\alpha})} \left(\frac{\mathrm{e}x}{\alpha}\right)^{\alpha} \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\mathrm{e}^{-kx}}{kx - \alpha} \quad (\tau \to \infty, 0 < \delta \leqslant x < \infty). \tag{2.9}$$

In the next sections we shall take a different approach, by using the theory of asymptotics of differential equations. We shall obtain improved approximations which (with the aid of the connection formula (1.5)) are uniformly valid for $0 \leqslant x < \infty$, and moreover are complete with explicit error bounds.

3. The Liouville–Green transformation

Considering again the differential equation (1.9), we shall derive Liouville–Green approximations directly from this equation. We first observe that the equation has regular singularities at $x = 0$ and $x = \pm(2k + 1)\pi\mathrm{i}$ ($k = 0, 1, 2, \ldots$). It also has an irregular singularity at $x = \infty$. Since we are only considering positive values of x, the complex poles are not of a direct concern to us, although we do note that they are infinite in number and the sequence of poles tends to the singularity at infinity in the complex x plane.

The appropriate general theory is given by Olver in [9, Chapter 6, Theorem 11.1], which provides Liouville–Green solutions compete with explicit error bounds. In order for these approximations to be uniformly valid at both $x=0$ and $x=\infty$ it turns out that we must rescale the independent variable in the following manner:

$$x = \tau\hat{x} \quad (\tau = \operatorname{Im}\alpha). \tag{3.1}$$

It will become clear later why this is required. On writing $w(x) = \hat{w}(\hat{x})$ we then express (1.9) in the form

$$\frac{\mathrm{d}^2\hat{w}}{\mathrm{d}\hat{x}^2} = \{\tau^2 f(\alpha,\hat{x}) + g(\hat{x})\}\hat{w}, \tag{3.2}$$

where

$$f(\alpha,\hat{x}) = \frac{1}{4} + \frac{\alpha^2}{4\tau^2\hat{x}^2} + \frac{(1-\alpha)\mathrm{e}^{\tau\hat{x}}}{2\tau\hat{x}(\mathrm{e}^{\tau\hat{x}}+1)} - \frac{1}{4(\mathrm{e}^{\tau\hat{x}}+1)^2}, \tag{3.3}$$

and

$$g(\hat{x}) = -\frac{1}{4\hat{x}^2}. \tag{3.4}$$

On referring to (1.4) it is readily verified that for τ large $f(\alpha,\hat{x})$ has no zeros on or near the real $\hat{x}$ axis, and therefore the differential equation (3.2) is free of turning points on the positive real $\hat{x}$ axis. Therefore asymptotic solutions only involve elementary functions. To obtain these solutions, we apply the well-known Liouville transformation, which involves a new independent variable defined by

$$\xi = \int f^{1/2}(\alpha,\hat{x})\,\mathrm{d}\hat{x}; \tag{3.5}$$

(see [9, Chapter 6, Section 1]). The square root branch is chosen so that

$$f^{1/2}(\alpha,\hat{x}) = \frac{1}{2} + \frac{1-\alpha}{2\tau\hat{x}} + \mathrm{O}\left(\frac{1}{\hat{x}^2}\right) \quad (\hat{x}\to\infty), \tag{3.6}$$

and by continuity for all other positive $\hat{x}$: in particular, from (3.3),

$$f^{1/2}(\alpha,\hat{x}) = -\frac{\alpha}{2\tau\hat{x}} - \frac{1-\alpha}{4\alpha} + \mathrm{O}(\hat{x}) \quad (\hat{x}\to 0). \tag{3.7}$$

We note in passing that the new variable ξ is complex, and before proceeding, we record the limit at the singular endpoints $\hat{x}=0$ and ∞. Firstly, assume that the integration constant in (3.5) is such that $\xi=0$ when $\hat{x}=a$, where $0<a<\infty$ can be arbitrarily assigned. We can then rewrite (3.5) in the form

$$\xi = \frac{\alpha}{2\tau}\int_{\hat{x}}^{a}\frac{1}{t}\,\mathrm{d}t - \int_{\hat{x}}^{a}\left\{f^{1/2}(\alpha,t) + \frac{\alpha}{2\tau t}\right\}\mathrm{d}t, \tag{3.8}$$

and consequently we find that

$$\xi = \frac{\alpha}{2\tau}\ln\left(\frac{a}{\hat{x}}\right) - c_1(\alpha) + \mathrm{O}(\hat{x}) \quad (\hat{x}\to 0), \tag{3.9}$$

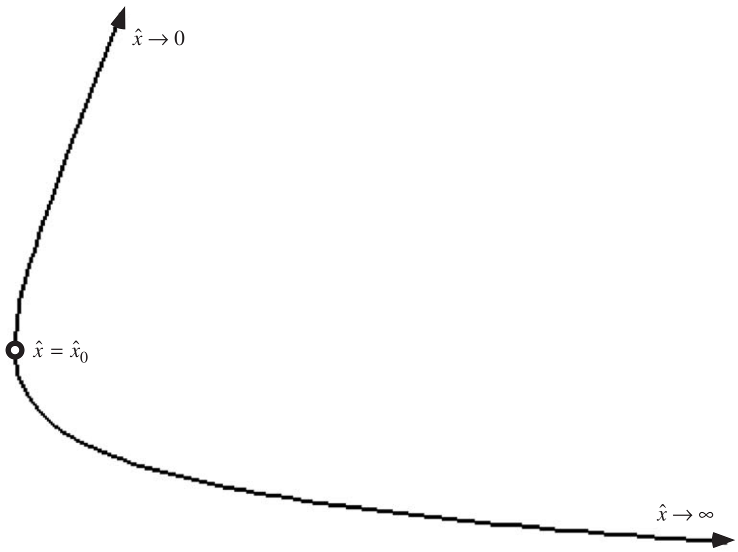

Fig. 2. Typical trajectory of $\xi(\hat{x})$ in the complex plane.

where

$$c_1(\alpha) = \int_0^a \left\{ f^{1/2}(\alpha, t) + \frac{\alpha}{2\tau t} \right\} \mathrm{d}t. \tag{3.10}$$

From (3.7) it follows that this integral converges at the lower limit.

Likewise, for the behaviour at $\hat{x} = \infty$, we express (3.5) in the form

$$\xi = \int_a^{\hat{x}} \left\{ \frac{1}{2} + \frac{1-\alpha}{2\tau t} \right\} \mathrm{d}t + \int_a^{\hat{x}} \left\{ f^{1/2}(\alpha, t) - \frac{1}{2} - \frac{1-\alpha}{2\tau t} \right\} \mathrm{d}t, \tag{3.11}$$

and as a result we deduce that

$$\xi = \frac{1}{2}(\hat{x} - a) + \frac{1-\alpha}{2\tau} \ln\left(\frac{\hat{x}}{a}\right) + c_2(\alpha) + \mathrm{O}\left(\frac{1}{\hat{x}}\right) \quad (\hat{x} \to \infty), \tag{3.12}$$

where

$$c_2(\alpha) = \int_a^{\infty} \left\{ f^{1/2}(\alpha, t) - \frac{1}{2} - \frac{1-\alpha}{2\tau t} \right\} \mathrm{d}t, \tag{3.13}$$

which converges at the upper limit on account of (3.6).

In Fig. 2 we show a typical trajectory of ξ where $\hat{x} \in (0, \infty)$ is regarded as a parameter, and $\alpha = \sigma + \mathrm{i}\tau$ is fixed.

The figure suggests that for each positive σ and τ, there exists a value $\hat{x}_0 \in (0, \infty)$ such that $\mathrm{Re}\,\xi$ is decreasing for $0 < \hat{x} < \hat{x}_0$ and increasing for $\hat{x}_0 < \hat{x} < \infty$. To confirm that this is indeed generally true, we first note from the definition (3.5) and a continuity argument that, for increasing positive $\hat{x}$, $\mathrm{Re}\,\xi$ changes from decreasing to increasing (or vice versa) when $\mathrm{Re}\, f^{1/2}(\alpha, \hat{x})$ has a simple zero (at $\hat{x} = \hat{x}_0$ say): the point(s) in question are those for which $\operatorname{Im} f(\alpha, \hat{x}_0) = 0$ with $\operatorname{Re} f(\alpha, \hat{x}_0) < 0$. Now, on setting $\alpha = \sigma + \mathrm{i}\tau$ in (3.3) we find that a unique $\hat{x}_0 \in (0, \infty)$ satisfying the requirements exists for each fixed positive σ and τ. In particular, using $\operatorname{Im} f(\alpha, \hat{x}_0) = 0$ we find that $\hat{x}_0$ is the solution of the following implicit equation

$$\tau \hat{x}_0 = \sigma(1 + \exp\{-\tau \hat{x}_0\}), \tag{3.14}$$

and using (3.5)–(3.7) we can confirm that $\operatorname{Re} \xi$ is decreasing for $0 < \hat{x} < \hat{x}_0$ and increasing for $\hat{x}_0 < \hat{x} < \infty$.

From (3.14) we can express $\hat{x}_0$ in the form

$$\hat{x}_0 = \tau^{-1} \Omega(\sigma), \tag{3.15}$$

where, in terms of the Lambert W function (see, for example, [13]),

$$\Omega(\sigma) = W(\sigma \mathrm{e}^{-\sigma}) + \sigma. \tag{3.16}$$

We remark that $\Omega(\sigma)$ is increasing for $\sigma > 0$, with $\Omega(0) = 0$, $\Omega(\frac{1}{2}) = 0.738835\ldots$, and $\Omega(1) = 1.27846\ldots$.

Having made the Liouville transformation, we now apply [9, Chapter 6, Theorem 11.1]. In doing so we identify Olver's z, $w(z)$ and $f(z)$ with our $\hat{x}$, $\hat{w}(\hat{x})$ and $\tau^2 f(\alpha, \hat{x})$, respectively. We take the so-called reference points of Olver's Theorem as $a_1 = 0$ and $a_2 = \infty$. Consider first the asymptotic solution of (3.2) which is to be recessive at $\hat{x} = 0$ (reference point $a_1 = 0$): since $\operatorname{Re} \xi = \infty$ when $\hat{x} = 0$ (see (1.4) and (3.9)) the required solution comes from [9, Chapter 6, Eq. (11.05)] with $j = 2$: on writing $\hat{w}^{(1)}(\alpha, \hat{x})$ and $\varepsilon^{(1)}(\alpha, \hat{x})$ for Olver's $w_2(z)$ and $\varepsilon_2(z)$, respectively, we thus obtain the following asymptotic solution of (3.2)

$$\hat{w}^{(1)}(\alpha, \hat{x}) = f^{-1/4}(\alpha, \hat{x}) \mathrm{e}^{-\tau\xi} \{1 + \varepsilon^{(1)}(\alpha, \hat{x})\}. \tag{3.17}$$

Consider now the error bounds [9, Chapter 1, Eq. (11.07)]. Using the definition of Olver's error-control function F, and the variational operator [9, Chapter 1, Eq. (11.02)], and recalling that $f(z)$ is to be replaced by $\tau^2 f(\alpha, \hat{x})$, we arrive at the following bounds corresponding to the reference point $a_1 = 0$,

$$\left|\varepsilon^{(1)}(\alpha, \hat{x})\right|, \left|\frac{1}{\tau f^{1/2}(\alpha, \hat{x})} \frac{\partial \varepsilon^{(1)}(\alpha, \hat{x})}{\partial \hat{x}}\right| \leqslant \exp\left\{\frac{1}{\tau} \int_0^{\hat{x}} |\Psi(\alpha, t) f^{1/2}(\alpha, t)| \, \mathrm{d}t\right\} - 1, \tag{3.18}$$

where

$$\Psi(\alpha, \hat{x}) = \frac{g(\hat{x})}{f(\alpha, \hat{x})} + \frac{4 f(\alpha, \hat{x}) f''(\alpha, \hat{x}) - 5 f'^2(\alpha, \hat{x})}{16 f^3(\alpha, \hat{x})}. \tag{3.19}$$

The bounds (3.18) are valid for $\operatorname{Re} \xi$ nonincreasing as $\hat{x}$ increases from $\hat{x} = 0$. Thus they hold uniformly for $0 \leqslant \hat{x} \leqslant \hat{x}_0$, where $\hat{x}_0$ is defined by (3.15) and (3.16): see also Fig. 2.

The second asymptotic solution of (3.2) is to be recessive at $\hat{x} = \infty$, and since $\operatorname{Re} \xi = \infty$ in this case too (see (3.12)) the required asymptotic solution also comes from setting $j = 2$ in [9, Chapter 6, Eq. (11.05)]: the difference is that the reference point is $a_2 = \infty$ rather than $a_1 = 0$. Thus, for this case, let us denote Olver's $w_2(z)$ and $\varepsilon_2(z)$ by $\hat{w}^{(2)}(\alpha, \hat{x})$ and $\varepsilon^{(2)}(\alpha, \hat{x})$, respectively. Then (3.2) possesses the following solution which is recessive at $\hat{x} = \infty$,

$$\hat{w}^{(2)}(\alpha, \hat{x}) = f^{-1/4}(\alpha, \hat{x}) \mathrm{e}^{-\tau\xi} \{1 + \varepsilon^{(2)}(\alpha, \hat{x})\}, \tag{3.20}$$

with the accompanying error bounds

$$|\varepsilon^{(2)}(\alpha,\hat{x})|, \left|\frac{1}{\tau f^{1/2}(\alpha,\hat{x})}\frac{\partial\varepsilon^{(2)}(\alpha,\hat{x})}{\partial\hat{x}}\right| \leqslant \exp\left\{\frac{1}{\tau}\int_{\hat{x}}^{\infty}|\Psi(\alpha,t)f^{1/2}(\alpha,t)|\,\mathrm{d}t\right\}-1. \tag{3.21}$$

These bounds are valid provided $\operatorname{Re}\xi$ is nonincreasing as $\hat{x}$ decreases from $\hat{x}=\infty$, and as such (3.21) holds uniformly for $\hat{x}_0 \leqslant \hat{x} < \infty$: see again Fig. 2.

Having constructed the Liouville–Green solutions, we conclude this section by examining their error bounds in some more detail. The main issue is convergence of the integrals in (3.18) and (3.21) at the singular endpoints $\hat{x}=0$ and $\hat{x}=\infty$. The chosen partition (3.3) and (3.4) ensures convergence at $\hat{x}=\infty$, since from (3.3)

$$f(\alpha,\hat{x}) \sim \frac{1}{4}+\frac{(1-\alpha)}{2\tau\hat{x}} \quad (\hat{x}\to\infty), \tag{3.22}$$

with this relation being twice differentiable and uniformly valid for $0<\delta\leqslant\tau<\infty$. From [9, Chapter 6, Section 4], and in particular Eq. (4.06) of that reference, we see from (3.4) and (3.22) that the variation in the error bound [9, Chapter 6, Eq. (11.07)], and equivalently the integral on the right-hand side of (3.21), converges at $\hat{x}=\infty$, uniformly for $0<\delta\leqslant\tau<\infty$.

Next, $\hat{x}=0$ is a regular singularity of (3.2), and the relevant information in this case is provided by [9, Chapter 6, Section 4.3] (with $a_2=0$ in the notation of this reference). Now from (3.3)

$$f(\alpha,\hat{x}) \sim \frac{\alpha^2}{4\tau^2\hat{x}^2} \quad (\hat{x}\to 0), \tag{3.23}$$

uniformly for $0<\delta\leqslant\tau<\infty$. Thus f has a double pole, and as Olver remarks, the variation in the error bound [9, Chapter 6, Eq. (11.07)] converges at a double pole of f provided g also has a double pole, with leading coefficient $-\frac{1}{4}$. From (3.4) we see that this indeed is the case, and hence the integral on the right-hand side of (3.18) converges at $\hat{x}=0$ (uniformly for $0<\delta\leqslant\tau<\infty$). We remark that the scaling (3.1) was necessary to be able to partition the right-hand side of the (transformed) equation in such a way that the error bounds could converge at *both* singularities.

Finally, let us estimate the integrals in (3.18) and (3.21). To do so, we find from (3.3) that

$$f(\alpha,\hat{x}) = \left(\frac{\hat{x}-(\alpha/\tau)}{2\hat{x}}\right)^2\left\{1+\mathrm{O}\left(\frac{\hat{x}}{\mathrm{e}^{\tau\hat{x}}}\right)\right\}, \tag{3.24}$$

uniformly for $0\leqslant\hat{x}<\infty$ and $0<\delta\leqslant\tau<\infty$. By noting that $\hat{x}\mathrm{e}^{-\tau\hat{x}}=\tau^{-1}(\tau\hat{x}\mathrm{e}^{-\tau\hat{x}})=\tau^{-1}\mathrm{O}(1)$ for $0\leqslant\hat{x}<\infty$, and recalling (1.4), we deduce that

$$f(\alpha,\hat{x}) = \left(\frac{\hat{x}-i}{2\hat{x}}\right)^2\left\{1+\mathrm{O}\left(\frac{1}{\tau}\right)\right\}, \tag{3.25}$$

uniformly for $0\leqslant\hat{x}<\infty$. Moreover, one can readily establish that this is twice differentiable, and hence inserting (3.25) and its differentiated forms, along with (3.4), into (3.19) we find that

$$\Psi(\alpha,\hat{x}) = \frac{\hat{x}(\hat{x}+2i)}{(\hat{x}-i)^4}\left\{1+\mathrm{O}\left(\frac{1}{\tau}\right)\right\}, \tag{3.26}$$

uniformly for $0\leqslant\hat{x}<\infty$, which combined with (3.25) yields the estimate

$$\int |\Psi(\alpha,\hat{x})f^{1/2}(\alpha,\hat{x})|\,\mathrm{d}\hat{x}=\int\frac{(\hat{x}^2+4)^{1/2}}{2(\hat{x}^2+1)^{3/2}}\,\mathrm{d}\hat{x}\left\{1+\mathrm{O}\left(\frac{1}{\tau}\right)\right\} \tag{3.27}$$

uniformly for $0\leqslant\hat{x}<\infty$. This incidentally confirms the convergence of the integrals in (3.18) and (3.21) at both singularities.

4. Liouville–Green approximations

We shall now identify the asymptotic solutions with the exact solutions of (3.2). We first consider those that are recessive at $\hat{x}=0$, and we immediately deduce that there exists a constant $C_1(\alpha)$ such that

$$(\tau\hat{x})^{(1-\alpha)/2}(\mathrm{e}^{\tau\hat{x}}+1)^{1/2}Z_1(\alpha,\tau\hat{x})=C_1(\alpha)\hat{w}^{(1)}(\alpha,\hat{x}). \tag{4.1}$$

Returning to the original variable x via (3.1), we deduce from (3.17) and (4.1) that

$$Z_1(\alpha,x)=C_1(\alpha)H(\alpha,x)\mathrm{e}^{-\tau\xi}\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}, \tag{4.2}$$

where

$$H(\alpha,x)=x^{(\alpha-1)/2}(\mathrm{e}^{x}+1)^{-1/2}h^{-1/4}(\alpha,x), \tag{4.3}$$

and

$$h(\alpha,x)=f(\alpha,\tau^{-1}x)=\frac{1}{4}+\frac{\alpha^2}{4x^2}+\frac{(1-\alpha)\mathrm{e}^{x}}{2x(\mathrm{e}^{x}+1)}-\frac{1}{4(\mathrm{e}^{x}+1)^2}. \tag{4.4}$$

Usually one would determine the constant of proportionality $C_1(\alpha)$ by comparing both sides of (4.1) as x approaches a singularity (in this case $x=0$). However, we shall take a different approach which results in a much simpler approximation. The key is that the derivative of $Z_1(\alpha,x)$ is an elementary function (see (1.2)). With this in mind, we differentiate both sides of (4.2) to yield

$$\frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)}\frac{x^{\alpha-1}}{\mathrm{e}^{x}+1}=C_1(\alpha)\frac{\mathrm{d}}{\mathrm{d}x}[H(\alpha,x)\mathrm{e}^{-\tau\xi}\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}]. \tag{4.5}$$

Then, using

$$\mathrm{d}\xi/\mathrm{d}x=\tau^{-1}h^{1/2}(\alpha,x), \tag{4.6}$$

(see (3.5) and (4.4)) we have for the right-hand side of (4.5)

$$\begin{aligned}C_1(\alpha)\frac{\mathrm{d}}{\mathrm{d}x}[H(\alpha,x)\mathrm{e}^{-\tau\xi}\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}]&=C_1(\alpha)\mathrm{e}^{-\tau\xi}H(\alpha,x)\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}h^{1/2}(\alpha,x)\\&\quad\times\left[\frac{H'(\alpha,x)}{H(\alpha,x)h^{1/2}(\alpha,x)}-1+\frac{\partial\varepsilon^{(1)}(\alpha,\hat{x})/\partial\hat{x}}{\tau f^{1/2}(\alpha,\hat{x})\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}}\right].\end{aligned} \tag{4.7}$$

Next, on referring back to (4.2), it follows from (4.5) and (4.7) that

$$\frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)}\frac{x^{\alpha-1}}{\mathrm{e}^x+1}=Z_1(\alpha,x)h^{1/2}(\alpha,x)\times\left[\frac{H'(\alpha,x)}{H(\alpha,x)h^{1/2}(\alpha,x)}-1+\frac{\partial\varepsilon^{(1)}(\alpha,\hat{x})/\partial\hat{x}}{\tau f^{1/2}(\alpha,\hat{x})\{1+\varepsilon^{(1)}(\alpha,\hat{x})\}}\right]. \tag{4.8}$$

Solving this for $Z_1(\alpha, x)$ gives the desired uniform asymptotic approximation. The analysis for $Z_2(\alpha, x)$ is similar, and finally using

$$h^{1/2}(\alpha,x)=\frac{x-\alpha}{2x}\left[1+\frac{2x(\mathrm{e}^x+\alpha)(\mathrm{e}^x+1)-x^2}{(x-\alpha)^2(\mathrm{e}^x+1)^2}\right]^{1/2}, \tag{4.9}$$

we arrive at our main result.

Theorem 4.1. *For* $j = 1, 2$

$$Z_j(\alpha,x)=\frac{(-1)^j}{(1-2^{1-\alpha})\Gamma(\alpha)}\frac{x^{\alpha}}{(x-\alpha)(\mathrm{e}^x+1)(1+\chi(\alpha,x))^{1/2}}\{1+\delta^{(j)}(\alpha,\hat{x})\}^{-1}, \tag{4.10}$$

where

$$\chi(\alpha,x)=\frac{2x(\mathrm{e}^x+\alpha)(\mathrm{e}^x+1)-x^2}{(x-\alpha)^2(\mathrm{e}^x+1)^2}, \tag{4.11}$$

$$\delta^{(j)}(\alpha,x)=-\frac{1}{2}-\frac{H'(\alpha,x)}{2H(\alpha,x)h^{1/2}(\alpha,x)}-\frac{\partial\varepsilon^{(j)}(\alpha,\hat{x})/\partial\hat{x}}{2\tau f^{1/2}(\alpha,\hat{x})\{1+\varepsilon^{(j)}(\alpha,\hat{x})\}}, \tag{4.12}$$

and $H(\alpha, x)$, $h^{1/2}(\alpha, x)$ *are given by* (4.3) *and* (4.4), *respectively. The error terms* $\varepsilon^{(j)}(\alpha, \hat{x})$ *and their derivatives are bounded by* (3.18) *and* (3.21).

From the error bounds (3.18) and (3.21) we know that the third term on the right-hand side of (4.12) is $\mathrm{O}(\tau^{-1})$ uniformly for $0 \leqslant x \leqslant \Omega(\sigma)$ $(j = 1)$ and $\Omega(\sigma) \leqslant x < \infty$ $(j = 2)$, where $\Omega(\sigma)$ is defined by (3.16). We now assert that:

Lemma 4.2.

$$\delta^{(j)}(\alpha,x)=\mathrm{O}(\tau^{-1}), \tag{4.13}$$

uniformly for $0 \leqslant x \leqslant \Omega(\sigma)$ $(j = 1)$ *and* $\Omega(\sigma) \leqslant x < \infty$ $(j = 2)$.

To prove this, we shall show that

$$-\frac{1}{2}-\frac{H'(\alpha,x)}{2H(\alpha,x)h^{1/2}(\alpha,x)}=\mathrm{O}\left(\frac{1}{\tau}\right), \tag{4.14}$$

uniformly for $0 \leqslant x < \infty$. To establish this fact, we first find from (4.3) that

$$\frac{H'(\alpha,x)}{H(\alpha,x)}=\frac{\alpha-1}{2x}-\frac{1}{2}+\frac{1}{2(\mathrm{e}^x+1)}-\frac{h'(\alpha,x)}{4h(\alpha,x)}. \tag{4.15}$$

Next, from (1.4) and (4.9), it is readily verified that

$$h^{1/2}(\alpha, x) = \frac{x-\alpha}{2x}\left\{1 + \mathrm{O}\left(\frac{1}{\tau}\right)\right\}, \tag{4.16}$$

uniformly for $0 \leqslant x < \infty$. Therefore, combining (4.15) and (4.16), and after some calculation, we arrive at the desired estimate

$$-\frac{1}{2} - \frac{H'(\alpha, x)}{2H(\alpha, x)h^{1/2}(\alpha, x)} = \frac{x}{2(x-\alpha)^2} + \mathrm{O}\left(\frac{1}{\tau}\right) = \mathrm{O}\left(\frac{1}{\tau}\right), \tag{4.17}$$

with both O terms being uniform for $0 \leqslant x < \infty$. The Lemma now follows.

An extension of our approximations for $Z_1(\alpha, x)$ and $Z_2(\alpha, x)$ to $0 \leqslant x < \infty$ is immediately achieved from the connection formula (1.5). Thus, for example, $Z_1(\alpha, x)$ can be represented for $\Omega(\sigma) \leqslant x < \infty$ by the relation $Z_1(\alpha, x) = \zeta(\alpha) - Z_2(\alpha, x)$, in which $\zeta(\alpha)$ can be approximated by the Riemann–Siegel formula (see [1,5]), and $Z_2(\alpha, x)$ approximated by (4.10).

Note that when $\zeta(\alpha) = 0$ we have from (1.14) and Theorem 4.1 that the eigenfunction $\phi(\alpha, x)$ has the asymptotic approximation

$$\phi(\alpha, x) = \frac{1}{(1-2^{1-\alpha})\Gamma(\alpha)} \frac{x^{(1+\alpha)/2}}{(x-\alpha)(\mathrm{e}^x + 1)^{1/2}(1+\chi(\alpha, x))^{1/2}}\left\{1 + \mathrm{O}\left(\frac{1}{\tau}\right)\right\}, \tag{4.18}$$

which is uniformly valid for $0 \leqslant x < \infty$. Moreover, the O term tends to zero both when $x \to 0$ and when $x \to \infty$.

5. Numerical calculations

We shall compute the relative errors $\eta^{(j)}(\alpha, x)$ $(j = 1, 2)$ defined by

$$Z_j(\alpha, x) = \frac{(-1)^j}{(1-2^{1-\alpha})\Gamma(\alpha)} \frac{x^\alpha}{(x-\alpha)(\mathrm{e}^x + 1)(1+\chi(\alpha, x))^{1/2}}\left\{1 + \eta^{(j)}(\alpha, x)\right\}. \tag{5.1}$$

We consider two values of α, α_1 and α_2, say, where

$$\alpha_1 = \tfrac{1}{2} + 100i, \tag{5.2}$$

for which

$$\zeta(\alpha_1) = (2.6926\cdots) - (0.020386\cdots)i, \tag{5.3}$$

and

$$\alpha_2 = \tfrac{1}{2} + (101.317851\cdots)i, \tag{5.4}$$

this being chosen as a zero of $\zeta(\alpha)$. Thus $Z_1(\alpha_2, x) = -Z_2(\alpha_2, x) = x^{(\alpha_2-1)/2}(\mathrm{e}^x + 1)^{-1/2}\phi(\alpha_2, x)$, where $\phi(\alpha, x)$ is the eigenfunction (recessive at both $x = 0$ and ∞) which has the uniform asymptotic approximation (4.18).

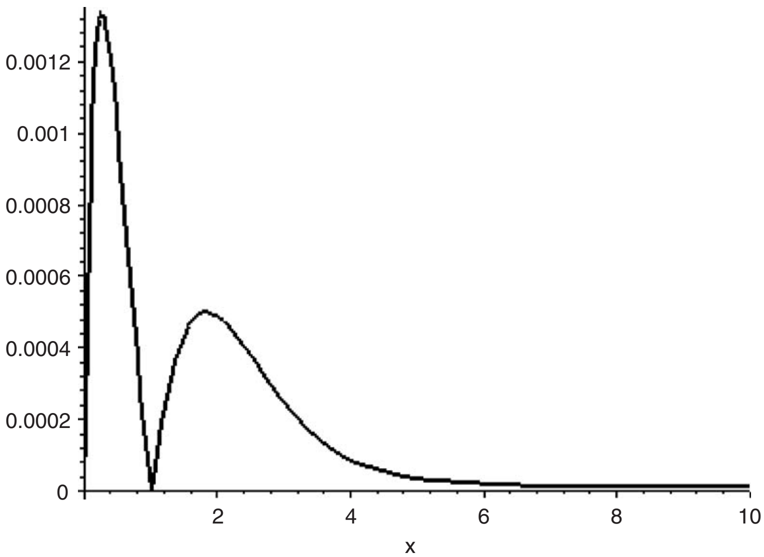

Fig. 3. Graph of the relative error $|\eta^{(1)}(\alpha_1, x)|$.

Table 1
Relative errors for various values of x

x	$\lvert\eta^{(1)}(\alpha_1, x)\rvert$	$\lvert\eta^{(2)}(\alpha_1, x)\rvert$	$\lvert\eta^{(j)}(\alpha_2, x)\rvert$
1.0E − 135	1.50008E − 137	1.23097E + 02	1.48057E − 137
1.0E − 132	1.50008E − 134	3.89266E + 00	1.48057E − 134
1.0E − 130	1.50008E − 132	3.89266E − 01	1.48057E − 132
1.0E − 125	1.50008E − 127	1.23097E − 03	1.48057E − 127
1.0E − 120	1.50008E − 122	3.89266E − 06	1.48057E − 122
1.0E − 03	1.49335E − 05	1.49335E − 05	1.47392E − 05
0.25	1.33196E − 03	1.33196E − 03	1.31464E − 03
$\Omega(0.5)$	4.60138E − 04	4.60138E − 04	4.54164E − 04
5	3.40746E − 05	3.40746E − 05	3.32888E − 05
10	1.01104E − 05	1.01104E − 05	9.72403E − 06
50	3.40608E − 05	3.40608E − 05	3.30506E − 05
100	2.84513E − 05	2.84513E − 05	2.80105E − 05
150	3.98908E − 02	1.78209E − 05	1.76874E − 05
155	5.96239E + 00	1.69896E − 05	1.68711E − 05
160	8.90997E + 02	1.62027E − 05	1.60974E − 05

In (5.1) we computed the exact value of $Z_1(\alpha, x)$ for small x by a Taylor series expansion, and the exact value of $Z_2(\alpha, x)$ for large x by the expansion (2.3): then $Z_1(\alpha_1, x)$ for large x and $Z_2(\alpha_1, x)$ for small x were computed via the connection formula (1.5).

The graph of $|\eta^{(1)}(\alpha, x)|$ for $0 < x \leqslant 10$ and $\alpha = \alpha_1$, is depicted in Fig. 3. This does not show the divergence as $x \to \infty$ because $|\eta^{(1)}(\alpha_1, x)|$ only becomes large when $x > 100$: this can be seen in Table 1 above, where we give values of $|\eta^{(1)}(\alpha_1, x)|$ and $|\eta^{(2)}(\alpha_1, x)|$ for various values of x. We also give values for $|\eta^{(j)}(\alpha_2, x)|$ (where $j = 1$ or 2, since both are equivalent on account of $\zeta(\alpha_2) = 0$). This error term vanishes at both $x = 0$ and ∞.

We also observe that the relative errors remain small in significantly larger intervals than the x intervals $[0, \Omega(\sigma)]$ and $[\Omega(\sigma), \infty)$ in which our explicit error bounds are valid. For example, the error bound for $|\eta^{(2)}(\alpha_1, x)|$ holds for $x \in [\Omega(\sigma), \infty)$, but this function only becomes large when x is exponentially small. To see why this is so in general, we first use (1.5) and (5.1) to derive the identity

$$\eta^{(2)}(\alpha, x) - \eta^{(1)}(\alpha, x) = (1 - 2^{1-\alpha})\Gamma(\alpha)x^{-\alpha}(x - \alpha)(\mathrm{e}^x + 1)(1 + \chi(\alpha, x))^{1/2}\zeta(\alpha). \tag{5.5}$$

Now, from Stirling's formula, we have

$$\Gamma(\alpha) = \Gamma(\sigma + \mathrm{i}\tau) \sim \sqrt{2\pi}\mathrm{e}^{-\pi\mathrm{i}/4}\left(\frac{\tau}{\mathrm{e}}\right)^{\mathrm{i}\tau}\mathrm{e}^{\sigma\pi\mathrm{i}/2}\tau^{\sigma-(1/2)}\mathrm{e}^{-\tau\pi/2} \quad (\tau \to \infty). \tag{5.6}$$

Hence, since $\chi(\alpha, x)$ is bounded (in fact $\mathrm{O}(\tau^{-1})$) for large τ uniformly for $0 \leqslant x < \infty$, we deduce that

$$\eta^{(2)}(\alpha, x) - \eta^{(1)}(\alpha, x) = \zeta(\alpha)\tau^{\sigma-(1/2)}\mathrm{e}^{-\tau\pi/2}x^{-\sigma}(x^2 + \tau^2)^{1/2}\mathrm{e}^x\mathrm{O}(1) \quad (\tau \to \infty, 0 < x < \infty). \tag{5.7}$$

Since it is well known that $\zeta(\sigma + \mathrm{i}\tau)$ has at worst algebraic growth as $\tau \to \infty$, it follows that

$$\eta^{(1)}(\alpha, x) = \eta^{(2)}(\alpha, x) + \mathrm{o}(1) \tag{5.8}$$

certainly for

$$\exp\left\{-\frac{\pi(1 - \kappa)\tau}{2\sigma}\right\} \leqslant x \leqslant \frac{1}{2}\pi(1 - \kappa)\tau, \tag{5.9}$$

where κ is an arbitrary small positive constant: in this interval the $\mathrm{o}(1)$ term in (5.8) is exponentially small in τ. This confirms our assertion above.

Returning to (4.10), we deduce that $\delta^{(1)}(\alpha, \hat{x}) = \mathrm{O}(\tau^{-1})$ uniformly for $0 \leqslant \hat{x} \leqslant \frac{1}{2}\pi(1-\kappa)$, and $\delta^{(2)}(\alpha, \hat{x}) = \mathrm{O}(\tau^{-1})$ uniformly for $\exp\{-\tau\pi(1 - \kappa)/(2\sigma)\} \leqslant \hat{x} < \infty$, in both cases $\kappa \in (0, 1)$ being arbitrary.

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